Abstract

High temperature metallic structural materials, such as Ni-base superalloys owe their strength to a two-phase microstructure consisting of an fcc matrix strengthened by intermetallic A3B type precipitates. The performance of these alloys derives from the exceptional high temperature strength of the L12-ordered A3B precipitate, which in turn is strongly influenced by planar faults created when the precipitate is sheared. *In this context, the broad goal of this work is to understand the role of composition on planar fault energies in A3B compounds with L12 structure.* Towards this aim, electronic structure calculations using density functional theory (DFT) was used to evaluate fault energies through direct simulations of faults and though indirect means involving analytical models. In the first part of the thesis, the effect of composition on the planar fault energies, elastic anisotropy, deformation modes and yield strength anomaly were explored in five pseudo-binaries (Ni, Co)3(Al,X) compositions of γ' (L12), where X = Ti, Ta, W, Ni. It was observed fault energies and deformation modes are sensitive to composition. The results are in good agreement with literature and can provide explanations for the deformation behaviour of both (Ni)3(Al, X) and Co3(Al,W). Though the results are encouraging, the above DFT calculations of fault energies are time-consuming, highlighting the need for high throughput models. In the second part of the thesis, such a model was developed to estimate these energies in well-known and novel A3B compositions. The new model treats the planar fault as a diffuse interface and allows estimation of fault energy in terms of energy of geometrically close packed structures with the same A3B composition and a bonding environment akin to that of the fault. The proposed model was used to predict energies of different superlattice faults in over 40 A3B compounds. The model was found to be highly accurate even without use of fitting parameters and has a fifteen-fold computational advantage over direct simulation. The model was extended to novel A3B compounds based on Pt3X, Rh3X and Ir3X where data is presently lacking. Despite the efficiency of the model, it had limitations in predicting fault energies in non-binary compositions. To account for this, in the last section of this thesis, a novel quasi-chemical model incorporating the far-field composition effects, was developed. The model was validated for several pseudo-binary systems and it was found that be more accurate than the diffuse interface model. The two models were then extended to predict fault energies in binary L12-ordered A3B compounds at high temperatures, complex multicomponent L12-ordered A3B compounds, and binary D019-ordered A3B compounds.